

=>

Uploading C:\Program Files\Stnexp\Queries\10781263.str



```
chain nodes :
1  3  4  6  7  8  9  17  30  34
ring nodes :
10 11 12 13 14 15 20 21 22 23 24 25 26 27 28 29
chain bonds :
1-3 1-6 1-9 3-4 6-7 6-8 9-12 17-34 28-30
ring bonds :
10-11 10-15 11-12 12-13 13-14 14-15 20-21 20-24 21-22 22-23 23-24 25-26
25-29 26-27 27-28 28-29
exact/norm bonds :
1-3 1-6 1-9 3-4 6-7 6-8 9-12 17-34 20-21 20-24 21-22 22-23 23-24 25-26
25-29 26-27 27-28 28-29 28-30
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 10 : 20 : 25 :
```

G1:[\*1],[\*2]

```
Connectivity :
4:1 E exact RC ring/chain 9:2 E exact RC ring/chain
Match level :
1:Atom 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom
13:Atom 14:Atom 15:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:CLASS 34:CLASS
Generic attributes :
1:
Saturation : Unsaturated
Number of Hetero Atoms : 2 or more
Type of Ring System : Polycyclic
17:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
```

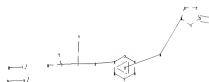
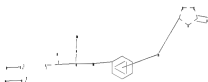
Element Count :  
 Node 1: Limited  
   C,C7  
   N,N2

Node 17: Limited  
   C,C6

L1       STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10781263-isoxazole.str



```
chain nodes :
1  3  4  6  7  8  16  24  25  26  30  31  32
ring nodes :
9  10 11 12 13 14 19 20 21 22 23
chain bonds :
1-3  1-8  1-31  3-4  6-31  7-24  8-11  16-20  23-32  25-26  30-31
ring bonds :
9-10  9-14  10-11  11-12  12-13  13-14  19-20  19-23  20-21  21-22  22-23
exact/norm bonds :
1-3  1-8  1-31  3-4  6-31  8-11  19-20  19-23  20-21  21-22  22-23  23-32  25-26
30-31
exact bonds :
7-24  16-20
normalized bonds :
9-10  9-14  10-11  11-12  12-13  13-14
isolated ring systems :
containing 9 : 19 :
```

G1:[\*1],[\*2]

Connectivity :  
 4:1 E exact RC ring/chain 8:2 E exact RC ring/chain 26:1 E exact RC ring/chain

Match level :

1:Atom 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom  
 12:Atom  
 13:Atom 14:Atom 16:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom  
 24:CLASS 25:CLASS  
 26:CLASS 30:CLASS 31:CLASS 32:CLASS

Generic attributes :

1:  
 Saturation : Unsaturated  
 Number of Hetero Atoms : 2 or more  
 Type of Ring System : Polycyclic  
 16:  
 Saturation : Unsaturated  
 Number of Carbon Atoms : less than 7  
 Type of Ring System : Monocyclic

Element Count :

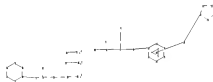
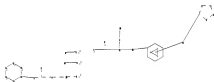
Node 1: Limited  
 C,C7  
 N,N2

Node 16: Limited  
 C,C6

L10 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10781263-tetrazole.str



chain nodes :

1 3 4 7 8 9 17 25 26 27 28 29 30 31 32 33 44

ring nodes :

6 10 11 12 13 14 15 20 21 22 23 24 34 35 36 37 38 39

```

chain bonds :
1-3 1-6 1-9 3-4 6-7 6-44 8-25 9-12 17-21 26-27 28-29 29-30 30-31 31-32
31-33 33-39
ring bonds :
6-45 10-11 10-15 11-12 12-13 13-14 14-15 20-21 20-24 21-22 22-23 23-24
34-35 34-39 35-36 36-37 37-38 38-39
exact/norm bonds :
1-3 1-6 1-9 3-4 6-7 6-45 6-44 9-12 20-21 20-24 21-22 22-23 23-24 26-27
28-29 29-30 30-31 31-32 31-33 33-39
exact bonds :
8-25 17-21 34-35 34-39 35-36 36-37 37-38 38-39
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 10 : 20 : 34 :

```

```
G1:[*1],[*2],[*3]
```

```

Connectivity :
4:1 E exact RC ring/chain 9:2 E exact RC ring/chain 27:1 E exact RC ring/chain
29:2 E exact RC ring/chain

```

```
Match level :
```

```

1:Atom 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom
13:Atom 14:Atom 15:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
24:Atom 25:CLASS
26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS
34:Atom 35:Atom
36:Atom 37:Atom 38:Atom 39:Atom 44:CLASS

```

```
Generic attributes :
```

```

1:
Saturation : Unsaturated
Number of Hetero Atoms : 2 or more
Type of Ring System : Polycyclic
17:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

```

```
Element Count :
```

```

Node 1: Limited
C,C7
N,N2

```

```

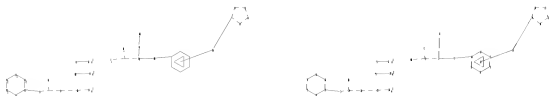
Node 17: Limited
C,C6

```

```
L11 STRUCTURE UPLOADED
```

```
=>
```

```
Uploading C:\Program Files\Stnexp\Queries\10781263-tetrazole-2.str
```



```

chain nodes :
1 3 4 6 7 15 23 24 25 26 27 28 29 30 31 41 42 44
ring nodes :
8 9 10 11 12 13 18 19 20 21 22 32 33 34 35 36 37
chain bonds :
1-3 1-7 1-41 3-4 6-23 7-10 15-19 24-25 26-27 27-28 28-29 29-30 29-31
31-37 41-42 41-44
ring bonds :
8-9 8-13 9-10 10-11 11-12 12-13 18-19 18-22 19-20 20-21 21-22 32-33
32-37
33-34 34-35 35-36 36-37
exact/norm bonds :
1-3 1-7 1-41 3-4 7-10 18-19 18-22 19-20 20-21 21-22 24-25 26-27 27-28
28-29 29-30 29-31 31-37 41-42 41-44
exact bonds :
6-23 15-19 32-33 32-37 33-34 34-35 35-36 36-37
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13
isolated ring systems :
containing 8 : 18 : 32 :

```

```
G1:[*1],[*2],[*3]
```

```

Connectivity :
4:1 E exact RC ring/chain 7:2 E exact RC ring/chain 25:1 E exact RC ring/chain
27:2 E exact RC ring/chain
Match level :
1:Atom 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom
13:Atom 15:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS
24:CLASS 25:CLASS
26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom 33:Atom
34:Atom 35:Atom
36:Atom 37:Atom 41:CLASS 42:CLASS 44:CLASS
Generic attributes :
1:
Saturation : Unsaturated
Number of Hetero Atoms : 2 or more
Type of Ring System : Polycyclic

```

15:  
 Saturation : Unsaturated  
 Number of Carbon Atoms : less than 7  
 Type of Ring System : Monocyclic

Element Count :

Node 1: Limited

C,C7

N,N2

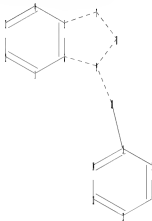
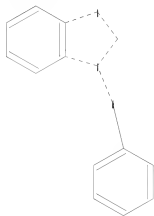
Node 15: Limited

C,C6

L14 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10781263-tetrazole-2-narrow.str



chain nodes :

10

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17

chain bonds :

9-10 10-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16

16-17

exact/norm bonds :

5-7 6-9 7-8 8-9 9-10 10-15

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

isolated ring systems :

containing 12 :

Connectivity :

10:2 E exact RC ring/chain

Match level :

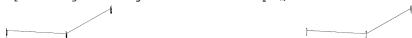
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L16      STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10781263-tetrazole-2-not-2.str



chain nodes :  
1 2 4  
chain bonds :  
1-2 2-4  
exact/norm bonds :  
1-2 2-4

Connectivity :  
4:2 M minimum RC ring/chain  
Match level :  
1:Atom 2:Atom 4:CLASS  
Generic attributes :  
2:  
Saturation : Unsaturated  
Type of Ring System : Monocyclic

Element Count :  
Node 2: Limited  
C,C1  
N,N4

L18      STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10781263-tetrazole-2-not-2.str



chain nodes :  
1 2 3  
chain bonds :  
1-2 1-3  
exact/norm bonds :  
1-2 1-3

Match level :  
1:Atom 2:Atom 3:Atom  
Generic attributes :  
1:  
Saturation : Unsaturated  
Type of Ring System : Monocyclic

Element Count :  
Node 1: Limited  
N,N4  
C,C1

L19       STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 10:35:41 ON 12 FEB 2008

L1           STRUCTURE UPLOADED

L2           10 S L1

L3           223 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:36:33 ON 12 FEB 2008

L4           1583 S L3

FILE 'STNGUIDE' ENTERED AT 10:36:43 ON 12 FEB 2008

FILE 'REGISTRY' ENTERED AT 10:37:38 ON 12 FEB 2008

L5           SCREEN 1842

L6           SCREEN 1844

L7           9 S L1 NOT L6 SAM

L8           189 S L1 NOT L6 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:38:21 ON 12 FEB 2008

L9           1582 S L8

FILE 'STNGUIDE' ENTERED AT 10:38:34 ON 12 FEB 2008

FILE 'REGISTRY' ENTERED AT 10:51:50 ON 12 FEB 2008  
SAV TEM L8 BRD781263/A

FILE 'STNGUIDE' ENTERED AT 10:52:12 ON 12 FEB 2008

FILE 'REGISTRY' ENTERED AT 10:56:14 ON 12 FEB 2008

L10          STRUCTURE UPLOADED

L11          STRUCTURE UPLOADED

L12          0 S L10 SAM SUB=L8

L13          9 S L10 SSS FULL SUB=L8

FILE 'STNGUIDE' ENTERED AT 10:57:23 ON 12 FEB 2008

FILE 'REGISTRY' ENTERED AT 10:59:22 ON 12 FEB 2008

L14          STRUCTURE UPLOADED

L15          118 S L14 SSS FULL SUB=L8

FILE 'STNGUIDE' ENTERED AT 11:00:23 ON 12 FEB 2008

FILE 'REGISTRY' ENTERED AT 11:01:35 ON 12 FEB 2008

FILE 'STNGUIDE' ENTERED AT 11:01:50 ON 12 FEB 2008

FILE 'REGISTRY' ENTERED AT 11:02:56 ON 12 FEB 2008

L16          STRUCTURE UPLOADED

L17          115 S L16 SSS FULL SUB=L15



FILE 'STNGUIDE' ENTERED AT 11:04:50 ON 12 FEB 2008

FILE 'REGISTRY' ENTERED AT 11:10:51 ON 12 FEB 2008

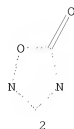
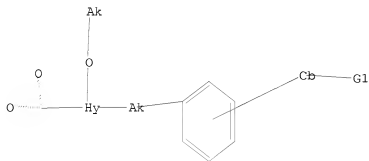
L18           STRUCTURE UPLOADED  
L19           STRUCTURE UPLOADED  
L20           53 S L18 SSS FULL SUB=L17  
L21           1 S L19 SSS FULL SUB=L17  
L22           62 S L17 NOT L20  
L23           61 S L22 NOT L21  
L24           70 S L13 OR L23  
              SAV TEM L24 NAR781263/A

FILE 'CAPLUS' ENTERED AT 11:12:39 ON 12 FEB 2008

L25           1575 S L24  
L26           1 S US2001-758355/APPS  
L27           1574 S L25 NOT L26

FILE 'REGISTRY' ENTERED AT 11:13:55 ON 12 FEB 2008

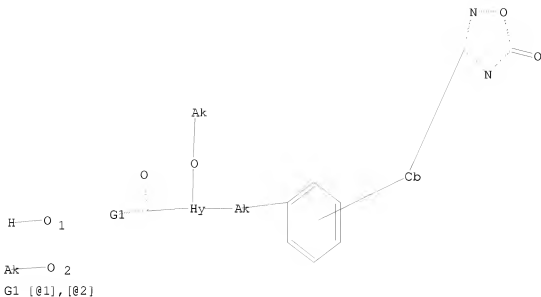
=> d 11  
L1 HAS NO ANSWERS  
L1           STR



G1 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> d 110  
L10 HAS NO ANSWERS  
L10           STR



Structure attributes must be viewed using STN Express query preparation.

=> d 111

L11 HAS NO ANSWERS

L11 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> d 114

L14 HAS NO ANSWERS

L14 STR

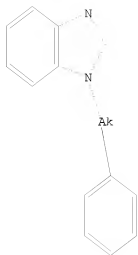
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> d 116

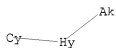
L16 HAS NO ANSWERS

L16 STR



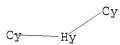
Structure attributes must be viewed using STN Express query preparation.

=> d 118  
 L18 HAS NO ANSWERS  
 L18 STR



Structure attributes must be viewed using STN Express query preparation.

=> d 119  
 L19 HAS NO ANSWERS  
 L19 STR



Structure attributes must be viewed using STN Express query preparation.